

LA-UR-18-22218

Approved for public release; distribution is unlimited.

Title: What is ENDF and NJOY? And why should I care?

Author(s): Haeck, Wim

Internal lab presentation, What is it? seminars for early career XCP

scientists

Issued: 2018-03-15





What is ENDF and NJOY?

And why should I care?



March 19, 2018



Not one but three questions ...

March 19, 2018

12-1 pm

TA03, Library, JRO1+2

- What is ENDF?
- What is NJOY?
- And why should I care?
- But I guess I will create even more ...



What is ENDF?

What is ENDF?

Easy answer: it's an acronym

ENDF = Evaluated Nuclear Data File/Format

Wait a minute, now I have more questions ...

- What is nuclear data?
- What does evaluated mean?
- Why distinguish File and Format?

What is nuclear data?

Nuclear data is everything we need to describe particle transport and nuclear processes

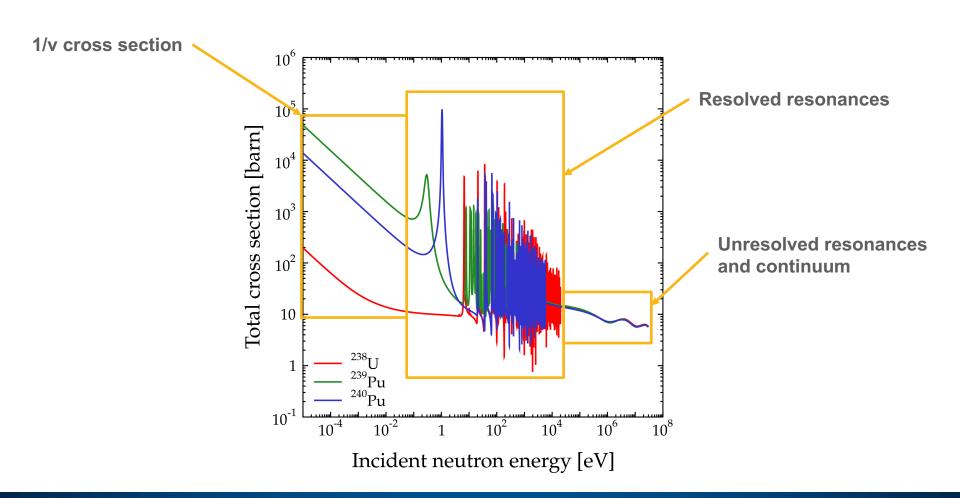
- Nuclear reaction data
 - Cross sections, secondary particle angular distributions, etc.
- Radioactive decay data
- Uncertainties (covariance data)

Used by particle simulation codes at LANL

- Monte Carlo particle transport with MCNP
- Deterministic particle transport with PARTISN
- Material irradiation with CINDER

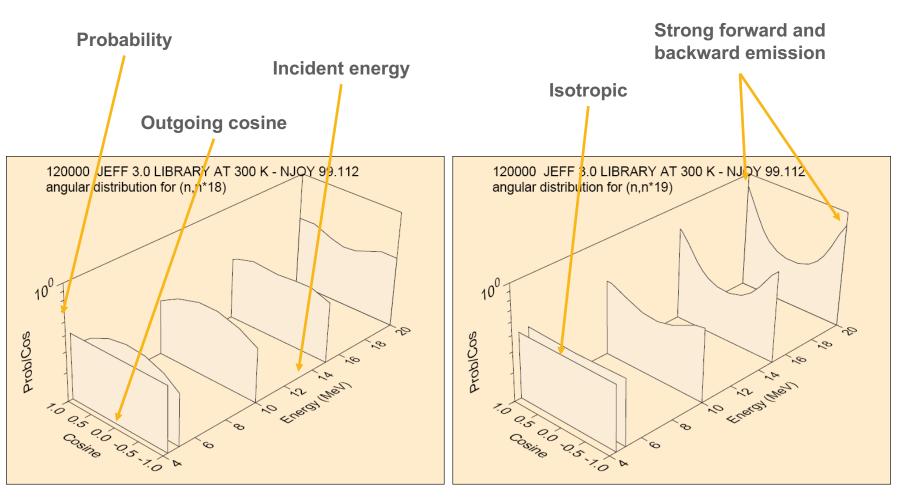
What is a cross section?

A cross section gives reaction probability



What is an angular distribution?

It gives the direction of the outgoing particle

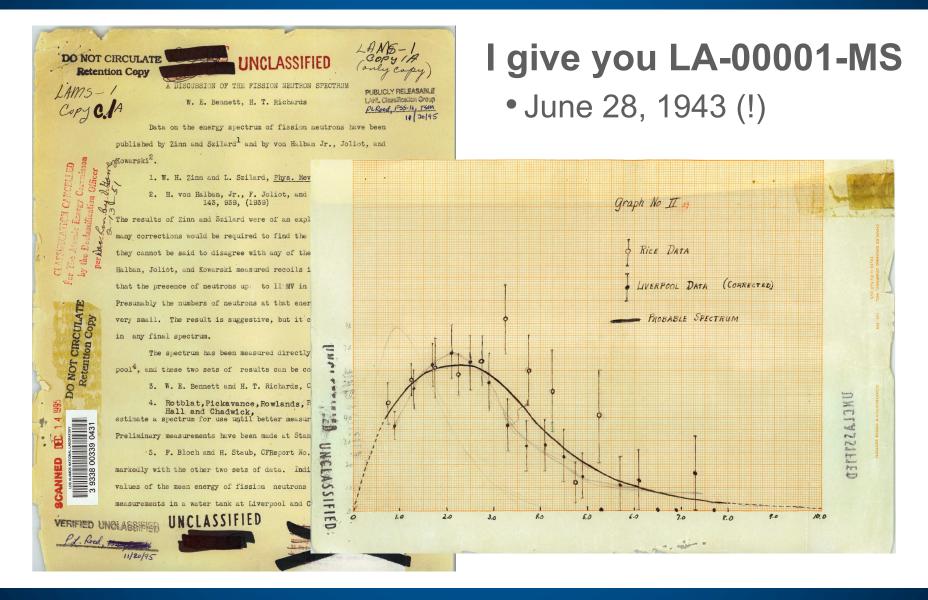


What does evaluated mean?

Evaluation is combining experimental data and nuclear interaction theory to provide the best available data and uncertainty in a common energy range

Maybe we need a "What is it, nuclear data evaluation?"

Can you give an example?



Why distinguish File and Format?

ENDF = Evaluated Nuclear Data File/Format

Evaluated Nuclear Data Format

- Format specification for storing/organising nuclear data
- Format versions are designated with an Arabic number
 - ENDF-6 is the current format version

Evaluated Nuclear Data File

- The name of the US nuclear data library
- Library versions are designated with a Roman numeral

ENDF/B-VIII.0 is the latest version, released in February 2018

Where does it come from?

ENDF was created in the mid-1960s

- The format has gone through 6 iterations
- Used for 8 generations of the ENDF/B library
 - ENDF/B-I in July 1968
 - ENDF/B-VIII.0 in February 2018

ENDF is developed and maintained by the **NNDC** and coordinated by **CSEWG**

- NNDC: National Nuclear Data Centre at BNL
- CSEWG: Cross Section Evaluation Working Group
 - Collaboration between national labs, universities and nuclear industry from the US and Canada

Does anybody else use it?

The ENDF format is the de facto standard for all nuclear data libraries in the world.

There are multiple "independent" libraries

- Europe: Joint European Fission and Fusion (JEFF)
- Japan: Japanese Evaluated Nuclear Data Library (JENDL)
- China: Chinese Evaluated Nuclear Data Library (CENDL)
- Russia: BROND
- All libraries are freely available from different nuclear data centres (OECD/NEA, IAEA/NDS, BNL/NNDC)

What does it look like?

```
9.223500+4 2.330248+2
                                                                  09228 3 18
                                                                                 1
1.934054+8 1.934054+8
                                                                8399228 3 18
                                                                                 2
       839
                                                                    9228 3 18
1.000000-5 \ 0.00000+00 \ 2.250000+3 \ 0.00000+00 \ 2.250000+3 \ 2.634378+09228 \ 3 \ 18
2.250014+3 2.668097+0 2.250056+3 2.769988+0 2.250112+3 2.907176+09228 3 18
2.250251+3 3.252747+0 2.250307+3 3.389935+0 2.250363+3 3.525523+09228 3 18
2.250419+3 3.658711+0 2.250470+3 3.778100+0 2.250517+3 3.884190+09228 3 18
2.250563+3 3.987480+0 2.250598+3 4.063173+0 2.250633+3 4.136965+09228 3 18
2.250668+3 4.209058+0 2.250703+3 4.279151+0 2.250738+3 4.347343+09228 3 18
2.250772+3 4.413436+0 2.250807+3 4.477529+0 2.250842+3 4.539621+09228 3 18
                                                                                10
```

If you can read this, you are ready to join the nuclear data team. Send an email to nucldata@lanl.gov to apply.

An ENDF library has multiple sub-libraries

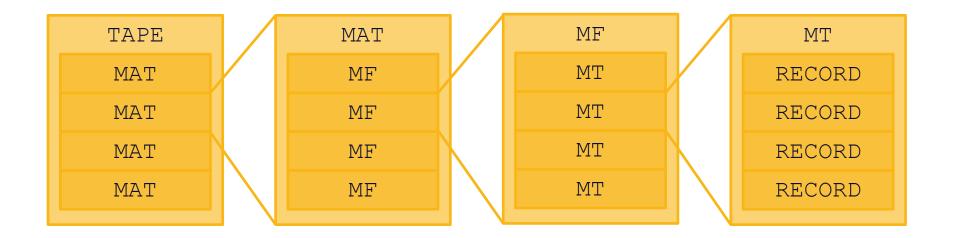
- Incident particle data: n, p, d, t, 3 He, α
- Thermal scattering data for crystals and molecules
- Radioactive decay data
- Neutron induced and spontaneous fission yields

Each sub-library is physically separated and stored in one or more "tapes"

ENDF jargon dating back to the time of magnetic tapes

Each tape is structured as a sequence

- Materials designated by the MAT number
- Files designated by the MF number
- Sections designated by the MT number
- A section is a sequence of records



A material is identified by its MAT number

- A specific nuclide, an element, a molecule, etc.
- Between 1 and 9999
- General rules for isotopes
 - Z * 100 + 25 for the first stable isotope
 - Decremented/incremented for the previous/next isotope
 - Numbers in between for metastable states
- For example:
 - 125 for H1, 9228 for U235
 - 9546 for Am242, 9547 for Am242m

Files identified by their MF number store specific types of data:

- MF1: descriptive and miscellaneous data
- MF2: resonance parameters
- MF3: cross section data
- MF4: secondary particle angular distribution
- MF5: secondary particle energy distribution
- MF6: correlated secondary particle angle-energy distribution
- MF31 to MF35: covariance data
- And there are even more ...

Sections designated by an MT number store specific "reaction data"

- These can be "simple" reactions
 - MT102 (neutron capture), MT51 to MT91 (inelastic levels)
- These can be "summation" reactions
 - MT4 (inelastic scattering, sum of MT51 to MT91)
- These can be "special" sections
 - MT451 (descriptive data, only in MF1)
 - MT151 (resonance parameters, only in MF2)

• MT numbers are limited to 1-999

Only 6 record types to store information:

- TEXT: stores just text
- CONT: 2 floating point numbers and 4 integers
- LIST: a list of values
- TAB1: a one dimensional function y = f(x)
- TAB2: a two dimensional function z = f(x,y), used in combination with multiple TAB1 records
- INTG: a correlation matrix (used for covariance data)

Special cases:

- HEAD: a CONT record at the beginning of each section
- TEND, MEND, FEND, SEND: records to signal the end of a tape, material, file and section

What does it look like?

Let's look at that again ...

```
9.223500+4 2.330248+2 0 0 0 0 0 09228 3 18 1
1.934054+8 1.934054+8 0 0 1 8399228 3 18 2
839 2 9228 3 18 3
1.000000-5 0.00000+00 2.250000+3 0.00000+00 2.250000+3 2.634378+09228 3 18 4
2.250014+3 2.668097+0 2.250056+3 2.769988+0 2.250112+3 2.907176+09228 3 18 5
2.250251+3 3.252747+0 2.250307+3 3.389935+0 2.250363+3 3.525523+09228 3 18 6
2.250419+3 3.658711+0 2.250470+3 3.778100+0 2.250517+3 3.884190+09228 3 18 7
2.250563+3 3.987480+0 2.250598+3 4.063173+0 2.250633+3 4.136965+09228 3 18 8
2.250668+3 4.209058+0 2.250703+3 4.279151+0 2.250738+3 4.347343+09228 3 18 9
2.250772+3 4.413436+0 2.250807+3 4.477529+0 2.250842+3 4.539621+09228 3 18
```

Lines consisting of 80 characters

- Six 11 characters columns for floats and integers
- Four columns for the MAT, MF, MT and sequence number

Isn't there anything better?

ENDF's structure is deceptively simple to understand but its content is extremely hard to master

GNDS = Generalised Nuclear Data Structure

- Initially developed at LLNL to replace ENDL
- Now an international collaboration through OECD/NEA
 - WPEC SG38, WPEC EG-GNDS, WPEC SG43
- A more physical approach to storing data
- This should eventually replace ENDF

Easy answer: it used to be an acronym ...

Multigroup Interpretation of Nuclear X sections

What do you mean: that's MINX, not NJOY?

40 years ago, there was this printer failure ...

- $\bullet M + 1 = N$
- $\bullet I + 1 = J$
- $\bullet N + 1 = 0$
- $\bullet X + 1 = Y$

It is LANL's nuclear data processing software

Initially developed in the '70s as a single package to replace all of LANL's previous tools

- Originally written in Fortran-77
- Known as MINX-II prior to the printer malfunction
- MINX: Multi-group Interpretation of Nuclear X sections
- LAPHAN0 for photon production
- GAMLEG for photon interaction data
- ETOPL for MCN (MCNP predecessor) libraries

NJOY was first released in 1977

- Last major releases in '99, 2012 and 2016
- NJOY evolves because ENDF evolves
- Still developed in Fortran ...

NJOY2016.29 is the latest version

- It is now open source software
- Available from https://github.com/njoy/NJOY2016

Similar tools exist

AMPX (ORNL), PREPRO (IAEA), Fudge (LLNL), etc.

What does it do?

NJOY provides a set of data processing modules that can be called sequentially

- RECONR: reconstruct and linearise cross section data
- BROADR: temperature dependent cross sections
- GROUPR: multi-group cross sections
- HEATR: calculate KERMA and DPA cross sections
- THERMR: thermal scattering data
- GASPR: charged particle production cross sections
- ACER: produce ACE libraries for MCNP
- PLOTR & VIEWR: visualisation of nuclear data

And there are many more modules ...

What does it look like?

```
moder
20 -25
reconr
-25 - 21
'AM241 - 293.6 K - JENDL 4.0 (NJOY 99.259)'/
9543 0 0
0.001 0 0.01 5e-08
0 /
broadr
-25 -21 -22
9543 1 0 0 0
0.001 1e+06 0.01 5e-08
293.6
0 /
heatr
-25 -22 -21 /
9543 5 0 0 0 0 /
302 318 402 442 444 /
thermr
0 -21 -22 /
0 9543 16 1 1 0 1 221 2 /
293.6
0.001 5.0
gaspr
-25 -22 -21 /
```

```
unresr
-25 -21 -22
9543 1 9 1
293.6
1e+10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1
0 /
purr
-25 -22 -21
9543 1 9 20 64 1 0
293.6
1e+10 1e+8 1e+6 1e+4 1e+3 3e+2 1e+2 3e+1 1e+1
0 /
acer
-25 -21 0 40 41
1 0 1 .02 /
'AM241 - 293.6 K - JENDL 4.0 (NJOY 99.259)'/
9543 293.6
1 1
acer
0 40 42 40 41
7 1 1 -1 /
'AM241 - 293.6 K - JENDL 4.0 (NJOY 99.259)'/
stop
```

Isn't there anything better?

NJOY21, NJOY for the 21st century

- Complete, ground-up rewrite of NJOY
- Modernization of code base
- Written in C++ using latest programming techniques
- Verified and validated
- Backwards compatible with NJOY2016

For more information:

- https://njoy.github.io/NJOY21
- https://github.com/njoy

Isn't there anything better?

Main goals for NJOY21

- Maintain NJOY's image of a trusted and stable processing code
 - Every function and feature is automatically, frequently, and regularly tested
 - Every feature of NJOY will be documented
- Easier to build, verify and validate, interact, process
- More flexible
- Faster
- More maintainable

And why should I care?

And why should I care?

Nuclear data has its uses ...

